

Theory for Electron-Doped Cuprate Superconductors: d -wave symmetry order parameter

D. Manske¹, I. Eremin², and K.H. Bennemann¹

¹*Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany*

²*Physics Department, Kazan State University, Kremlyovskaya 18, 420008 Kazan, Russia*
(February 1, 2008)

Using as a model the Hubbard Hamiltonian we determine various basic properties of electron-doped cuprate superconductors like $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$ and $\text{Pr}_{2-x}\text{Ce}_x\text{CuO}_4$ for a spin-fluctuation-induced pairing mechanism. Most importantly we find a narrow range of superconductivity and like for hole-doped cuprates $d_{x^2-y^2}$ -symmetry for the superconducting order parameter. The superconducting transition temperatures $T_c(x)$ for various electron doping concentrations x are calculated to be much smaller than for hole-doped cuprates due to the different Fermi surface and a flat band well below the Fermi level. Lattice disorder may sensitively distort the symmetry $d_{x^2-y^2}$ via electron-phonon interaction.

74.25.Dw, 74.20.Mn, 74.25.-q, 74.72.-h

One expects on general physical grounds if Cooper-pairing is controlled by antiferromagnetism that d -wave symmetry pairing should also occur for electron-doped cuprates [1]. Until recently [3–5] experiment did not clearly support this and reported mainly s -wave pairing [6–8]. Maybe as a result of this, so far electron-doped cuprates received much less attention than hole-doped cuprates. Previously, we were rather successful in determining the doping dependence of antiferromagnetism in both electron- and hole-doped cuprates by using the Hubbard Hamiltonian [9]. Applying this model to the hole-doped cuprates, many physical quantities like the normal-state pseudogap and the doping dependence of T_c can also be described [10,11].

Hence, to get an uniform theory we use here for the superconducting properties of electron-doped cuprates also as a model the 2D one-band Hubbard Hamiltonian

$$H = - \sum_{\langle ij \rangle \sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad . \quad (1)$$

Here, $c_{i\sigma}^\dagger$ creates an electron with spin σ on site i , U denotes the on-site Coulomb interaction, and t_{ij} is the hopping integral. For the optimally doped NCCO the dispersion ϵ_k and Fermi surface are taken in accordance with photoemission (ARPES) experiments [12]. Thus, we choose the parameters $t = 138$ meV and $t' = 0.30$ in calculating

$$\epsilon_k = -2t [\cos k_x + \cos k_y - 2t' \cos k_x \cos k_y + \mu/2] \quad , \quad (2)$$

where the chemical potential μ describes the band filling. Here and in the following, we set the lattice constant $a = b$ equal to unity.

In Fig. 1 the results for ϵ_k are shown. For comparison, the results of a tight-binding calculation with $t = 250$ meV and $t' = 0$, which is often used to describe the hole-doped superconductors, is also displayed. One immediately sees one important difference: in the case of

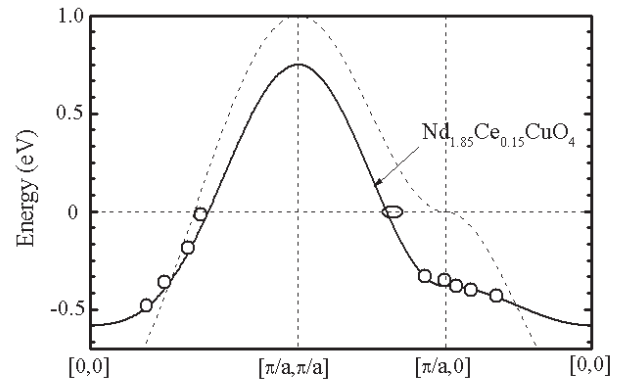


FIG. 1. Comparison of the energy dispersion ϵ_k for electron-doped cuprates and for hole-doped ones. Data (open dots) are taken from Ref. [12]. The solid curve refers to our tight-binding calculation as described in the text. The dashed curve corresponds to Eq. (2) with $t = 250$ meV and $t' = 0$.

NCCO the flat band is approximately 300 meV below the Fermi level, whereas for the hole-doped case the flat band lies very close to it. Thus, one expects a smaller T_c for electron-doped cuprates than for the hole-doped cuprates. Then, using ϵ_k in a spin-fluctuation-induced pairing theory in the framework of the so-called FLEX approximation [13–15], we calculate the doping dependence $T_c(x)$ and some other basic properties.

In Fig. 2 we show results for the real part of the spin susceptibility at 100K in the weak-coupling limit for $\omega = 0$ (solid curve) and for $\omega = \omega_{sf} \approx 0.47t$ (dashed curve). ω_{sf} denotes the spin fluctuation (paramagnon) energy, where a peak in $\text{Im } \chi(\mathbf{Q}, \omega)$ occurs. The commensurate structure of $\text{Re } \chi(\mathbf{q}, \omega = 0)$ is in accordance with recent calculations in Ref. [16], where it was pointed out that the exchange of spin fluctuations yield a good description of the normal state Hall coefficient R_H for both hole- and electron-doped cuprates. Furthermore, we also

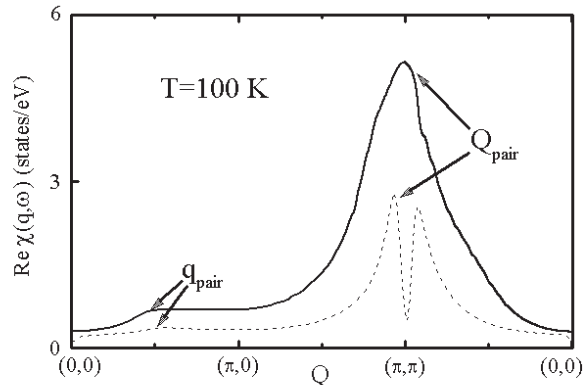


FIG. 2. Momentum dependence of the real part of the spin susceptibility along the BZ route $(0,0) \rightarrow (\pi,0) \rightarrow (\pi,\pi) \rightarrow (0,0)$ at $T = 100$ K for $\omega = 0$ (solid curve) and $\omega = \omega_{sf} \approx 0.47t$ (dashed curve). The main contributions to the corresponding pairing interaction come from \mathbf{q}_{pair} (along the anti-nodes) and \mathbf{Q}_{pair} (along the 'hot spots') as is illustrated in Fig. 5.

find a linear temperature dependence of the in-plane resistivity $\rho_{ab}(T)$, if we do not take into account an additional electron-phonon coupling. This will be discussed later. Concerning the superconducting properties, it was stated in Ref. [17] that in contrast to the hole-doped superconductors the electron-doped systems may be also close to a d_{xy} -symmetry instability. However, within the picture of a spin-fluctuation-induced pairing this is definitely not the case. Since the lower tiny peak favors d_{xy} pairing symmetry and the dominating larger peak $d_{x^2-y^2}$ symmetry (but is pair-breaking for d_{xy} -symmetry), one understands why an underlying superconducting order parameter $\phi(\mathbf{k},\omega)$ exhibits almost pure $d_{x^2-y^2}$ symmetry.

In Fig. 3 we present our result for $\phi(\mathbf{k},\omega)$ for $\omega = 0$ and a doping $x = 0.15$ at $T/T_c = 0.8$, where the gap has just opened. The gap function has clearly $d_{x^2-y^2}$ -wave symmetry. This is in agreement with the reported linear dependence of the in-plane penetration depth for low temperatures [4,5] and with phase-sensitive measurements [3]. From our obtained result of a pure $d_{x^2-y^2}$ -wave superconducting order parameter we expect a zero-bias conductance peak (ZBCP) [18] as observed for the hole-doped superconductors [7]. However, its absence in the electron-doped cuprates may be attributed to small changes in the surface quality and roughness [19] or to disorder [20]. Note, the incommensurate structure in the order parameter close to $(\pi,0)$ results from the double peak structure in $\text{Re } \chi$ at $\omega \approx \omega_{sf} = 0.47t$ shown in Fig. 2. Physically, it means that Cooper-pairing occurs not only for $\mathbf{Q} = (\pi,\pi)$, but mostly for $\omega = \omega_{sf}$ and for $\mathbf{Q}^* = (\pi - \delta, \pi + \delta)$. Furthermore, from Fig. 2, Fig. 3,

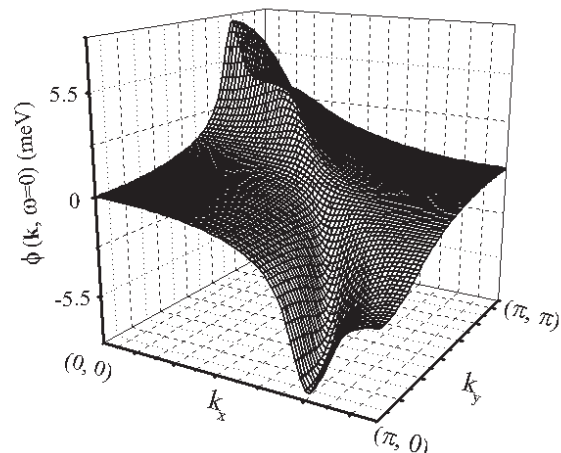


FIG. 3. Calculated $d_{x^2-y^2}$ -wave symmetry of the superconducting order parameter at $T/T_c=0.8$ for $x=0.15$ in the first square of the Brillouin Zone.

and Fig. 5 we conclude that *no* d_{xy} -symmetry component is present in the superconducting order parameter, since the dominating $d_{x^2-y^2}$ -type pairing suppresses d_{xy} pairing. ARPES study might test this.

In Fig. 4 we present our results for the phase diagram $T_c(x)$ and $T_N(x)$. We find that in comparison to hole-doped superconductors smaller T_c values and superconductivity in a narrower doping range as is also observed in experiment [21]. Responsible for this are poorer nesting properties of the Fermi surface and a flat band around $(\pi,0)$ which lies well below the Fermi level. The narrow doping range is due to antiferromagnetism up to $x = 0.13$ and, for increasing x , rapidly decreasing nesting properties. We have calculated the Cooper-pair coherence length ξ_0 , i.e. the size of a Cooper-pair, and find similar values for electron-doped and hole-doped superconductors (from 6 Å to 9 Å). If due to strong coupling lifetime effects the superfluid density n_s becomes small, the distance d between Cooper pairs increases. If for $0.15 > x > 0.13$ the Cooper-pairs do not overlap significantly, i.e. $d/\xi_0 > 1$, then Cooper-pair phase fluctuations get important [23,24,11]. Thus we expect like for hole-doped superconductors $T_c \propto n_s$. Assuming that n_s increases approximately linearly from $x \approx 0.13$ to $x \approx 0.15$ we estimate a T_c which is smaller than calculated from $\phi(\mathbf{k},\omega) = 0$ (see Fig. 4). As a consequence more experiments determining T_c for $x \leq 0.15$ should be performed to check on the Uemura scaling $T_c \propto n_s$.

The effect of electron-lattice coupling on superconductivity should depend on lattice perturbations like oxygen deficiencies. Then, the isotope effect may show a distinct effect of electron-phonon coupling on T_c . On general grounds we expect a weakening of the $d_{x^2-y^2}$ -pairing symmetry if we include the electron-phonon interaction and if this plays a significant role. The absence of an isotope effect ($\alpha_0 = d \ln T_c / d \ln M \approx 0.05$)

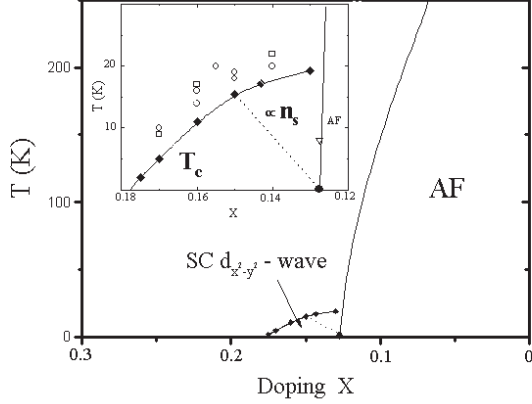


FIG. 4. Phase diagram $T(x)$ for electron-doped cuprates. The AF transition line is taken from Ref. [9]. Inset: blow-up of the doping region $0.18 < x < 0.12$. The solid curve corresponds to our calculated T_c values obtained from $\phi(\mathbf{k}, \omega) = 0$. For a comparison, also experimental data are shown (squares from Ref. [22], circles from Ref. [25], triangle from [26]). The dotted curve refers to $T_s \propto n_s$.

for doping $x = 0.15$ (see Ref. [27]) suggests the presence of a pure $d_{x^2-y^2}$ -symmetry. We know from Fig. 2 that phonons connecting the Fermi surface with wave vector $\mathbf{Q}_{\text{pair}} = (\pi, \pi)$ will add destructively to the spin fluctuation pairing [28]. If, due to exchange of spin fluctuations, a $d_{x^2-y^2}$ -symmetry instability is the dominant contribution to the pairing interaction, an additional electron-phonon coupling with wave vector $\mathbf{q}_{\text{pair}} = (0.5\pi, 0)$ would be also pair building. Note, we generally expect that due to the poorer nesting the pairing instability due to electron-phonon and spin fluctuation interaction become more easily comparable. In this case, the electron-phonon coupling would definitely favor s -wave symmetry of the underlying superconducting order parameter. This can be analyzed in detail by adding a term $\alpha^2 F(q, \omega)$ to the pairing interaction [28]. The corresponding phonon modes were calculated in Ref. [29]. Moreover, the inclusion of an electron-phonon interaction yields a quadratic term in the resistivity for lower temperatures [28] as it is observed in experiment [30].

To continue the discussion why the symmetry of the order parameter depends for electron-doped cuprates more sensitively on electron-phonon interaction, we show in Fig. 5 the calculated Fermi surface for optimally doped NCCO. Note, the topology of the Fermi surface for the electron-doped cuprates is very similar to optimally hole-doped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ (Bi2212) as it was also pointed out recently in Ref. [31]. We estimate that mainly no phonons are present along the edges $(-0.25\pi, \pi) \rightarrow (0.25\pi, \pi)$ bridging BZ areas, where the superconducting order parameter, $\phi(\mathbf{k}, \omega)$, is always positive (denoted by $+/+$). Note, attractive electron-phonon coupling brid-

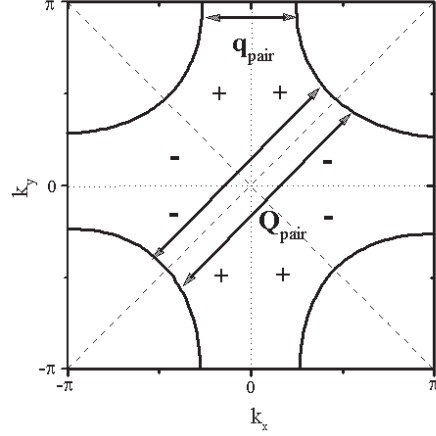


FIG. 5. Calculated Fermi surface for (optimally doped) NCCO. The $+/(-)$ sign and the dashed curve corresponds to the calculated momentum dependence (see Fig. 3) of the $d_{x^2-y^2}$ gap function $\phi(k, \omega = 0)$ and its nodes, respectively.

ing $+/(-)$ areas $(-0.5\pi, -0.5\pi) \rightarrow (0.5\pi, 0.5\pi)$ is *destructive* for $d_{x^2-y^2}$ Cooper pairing. However, due to poorer nesting conditions, pairing transitions of the type $+/(-)$ are somewhat contributing and then a mixed symmetry $\{d_{x^2-y^2} + \alpha s\}$ may occur.

Further experimental study of the doping dependence of the oxygen-isotope effect are necessary for a better understanding of the role played by the electron-phonon interaction. For example, if due to structural distortion and oxygen deficiency in the CuO_2 -plane the phonon spectrum $F(q, \omega)$ changes significantly, then this affects α_0 and reduces T_c . Possibly the reported large isotope effect of $\alpha_0 = 0.15$ for slightly changed oxygen content, i.e. $\text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_{3.8}$, could be related to this [32,33]. As an example, one might think of the oxygen out of plane B_{2u} mode, which become active if O_4 is replaced by $\text{O}_{3.8}$ [29].

In summary, our model for electron-doped cuprates yields like for hole-doped case pure $d_{x^2-y^2}$ symmetry pairing in a good agreement with recent experiments. In contrast to hole-doped superconductors, we find for electron-doped cuprates smaller T_c values due to a flat band dispersion around $(\pi, 0)$ well below the Fermi level. Furthermore, superconductivity only occurs for a narrow doping range $0.18 > x > 0.13$ because of the onset of antiferromagnetism, and, on the other side, due to poorer nesting conditions. We get $2\Delta/k_B T_c = 5.3$ for $x = 0.15$ in reasonable agreement with Ref. [6]. We argue that if the electron-phonon coupling becomes important, for example due to oxygen deficiency, then the s -wave pairing instability competes with $d_{x^2-y^2}$ -wave symmetry. This might explain a possible s -wave order parameter as reported in earlier measurements.

It's pleasure to thank R. Hackl, M. Opel, L. Alff, K. Scharnberg, and T. Dahm for useful discussions. One of

us (I. E.) would like to thank for the financial support German Academic Exchange Service (DAAD), the Freie Universität Berlin and Russian Scientific Council on Superconductivity (Grant No. 98014).

-
- [1] If the dominant *repulsive* pairing contribution in high- T_c superconductors can be mainly described by their spin susceptibility, then the underlying order parameter must change its sign. From group theory we know [2] that for a nested Fermi surface described by $\mathbf{Q} = (\pi, \pi)$, i.e. $\epsilon_{\mathbf{k}+\mathbf{Q}} = -\epsilon_{\mathbf{k}}$, the $d_{x^2-y^2}$ -symmetry order parameter is the simplest possibility.
 - [2] M. Sigrist and T. M. Rice, Z. Phys. B - Condensed Matter **68**, 9 (1987).
 - [3] C. C. Tsuei and J. R. Kirtly, cond-mat/0002341.
 - [4] J. David Kokales *et al.*, cond-mat/0002300.
 - [5] R. Prozorov, R. W. Gianetta, P. Fournier, and R. L. Greene, cond-mat/0002301.
 - [6] B. Stadlober *et al.*, Phys. Rev. Lett. **74**, 4911 (1995).
 - [7] L. Alff *et al.*, Phys. Rev. B. **58**, 11197 (1998).
 - [8] S. M. Anlage *et al.*, Phys. Rev. B. **50**, 523 (1994).
 - [9] G. Baumgärtel, J. Schmalian, and K. H. Bennemann, Phys. Rev. B **48**, 3983 (1993).
 - [10] T. Dahm, D. Manske, and L. Tewordt, Phys. Rev. B **55**, 15274 (1997).
 - [11] D. Manske, T. Dahm, and K. H. Bennemann, cond-mat/9912062.
 - [12] D. M. King *et al.*, Phys. Rev. Lett. **70**, 3159 (1993).
 - [13] N. E. Bickers, D. Scalapino, and S. R. White, Phys. Rev. Lett. **62**, 961 (1989).
 - [14] T. Dahm, and L. Tewordt, Phys. Rev. Lett. **74**, 793 (1995).
 - [15] M. Langer, J. Schmalian, S. Grabowski, and K.-H. Bennemann, Phys. Rev. Lett. **75**, 4508 (1995).
 - [16] H. Kontoni, K. Kanki, and K. Ueda, Phys. Rev. B **59**, 14723 (1999).
 - [17] K. Kuroki and H. Aoki, J. Phys. Soc. Jpn. **67**, 1533 (1998).
 - [18] M. Fogelstrom, D. Reiner, and J. A. Sauls, Phys. Rev. Lett. **79**, 281 (1997).
 - [19] J. A. Appelbaum, Phys. Rev. **154**, 633 (1967).
 - [20] M. Aprili, M. Covington, E. Paraoani, B. Niedermeier, and L. H. Greene, Phys. Rev. B **57**, 8139 (1998).
 - [21] C. Almasan, and M. B. Maple, in *Chemistry of High-Temperature Superconductors*, ed. by C. N. R. Rao (World Scientific, Singapore), 1991.
 - [22] E. F. Paulus *et al.*, Solid State Comm. **73**, 791 (1990).
 - [23] B. K. Chakraverty, A. Taraphder, and M. Avignon, Physica C **235-240**, 2323 (1994).
 - [24] V. J. Emery and S. A. Kivelson, Nature **374**, 434 (1995).
 - [25] H. Takagi, S. Uchida, and Y. Tokura, Phys. Rev. Lett. **62**, 1197 (1989).
 - [26] G. Liang *et al.*, Phys. Rev. B **40**, 2646 (1989).
 - [27] B. Batlogg *et al.*, Physica C **185-189**, 1385 (1991).
 - [28] T. Dahm, D. Manske, D. Fay, and L. Tewordt, Phys. Rev. B **54**, 12006 (1996).
 - [29] E. T. Heyen *et al.*, Solid State Comm. **74**, 1299 (1990).
 - [30] J. L. Peng, E. Maiser, T. Venkatesan, R. L. Greene, and G. Czyzek, Phys. Rev. B **55**, 6145 (1997).
 - [31] T. Tohoyama and S. Maekawa, Supercond. Sci. Technol. **13**, R17 (2000).
 - [32] J. P. Franck, in *Physical properties of High Temperature Superconductors*, ed. D. Ginsberg, (World Scientific, Singapore), 1994.
 - [33] M. Onada, S. Kondoh, and M. Sato, Solid State Comm. **70**, 1141 (1989).